Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

QMC Calculation of the Electronic Correlations in a Fullerene Molecule FEI LIN, JURIJ SMAKOV, ERIK SORENSEN, CATHERINE KALLIN, JOHN BERLINSKY, McMaster University, Hamilton, Ontario, Canada — Electronic energies are calculated for a Hubbard model on a fullerene molecule (C_{60}, C_{36} and C_{20}) using projector quantum Monte Carlo (QMC). Calculations are performed to accuracy high enough to determine the pair binding energy for two electrons added to neutral molecule. The method itself is checked against a variety of other quantum Monte Carlo methods as well as exact diagonalization for smaller molecules. We will also show the comparison of our results with the Hund's rule.

Fei Lin
Physics and Astronomy Department, McMaster University
Hamilton, Ontario, Canada

Date submitted: 22 Nov 2004 Electronic form version 1.4